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Implementing an aerosol dynamic shape factor for cerium oxide powder

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SUMMARY

The shape factor (X_B) of bulk powder CeO_2 (cerium oxide) particles (American Elements 2014) is estimated to be $X_B = 1.34$ (dimensionless). This is defined in relation to the measured aerated bulk density (0.91 g cm^{-3} , Hosokawa Micron, Summit NJ, 2018) of the CeO_2 powder. This information is used to determine the RRF (respirable release factor), and other parameters during drop test experiments of nuclear material storage containers at Los Alamos National Laboratory.

The calculation is based on an experimental shape factor ($X_p = 2.66$ dimensionless) for CeO_2 particles of the same (chain aggregate) morphology studied by other researchers (Brockmann and Rader 1990). In that work, the shape factor was defined in terms of the maximum possible (compacted) density of CeO_2 material (7.13 g cm^{-3}).

INTRODUCTION

The CeO_2 powder (Figure 1) for Brockmann and Rader's work (1990) and for this document (Figure 2) are large micron-sized agglomerates that are composed of many nanometer-sized subparticles. Brockmann and Rader (1990) measured the dynamic shape factor of CeO_2 particles based on a particle density of 7.13 g/cc of material. This is a maximum possible density for CeO_2 , with no assumed voids in the material sample. In their work, they were measuring chain aggregate particulates that they described as "compact clusters of material between 0.5 and a few micrometers in linear dimension" (Figure 1).

In comparison to the physical CeO_2 density of 7.13 g/cc (Brockmann and Rader 1990), the CeO_2 powder in this study has a measured aerated bulk density of 0.91 g/cc (Hosokawa Micron, Summit NJ, 2018). The current study does not describe CeO_2 powder as a compacted material with no internal voids, but utilizes the aerated bulk density (ρ_B) as a standard measurement (ASTM 2018) that accounts for material properties of non-compacted powders.

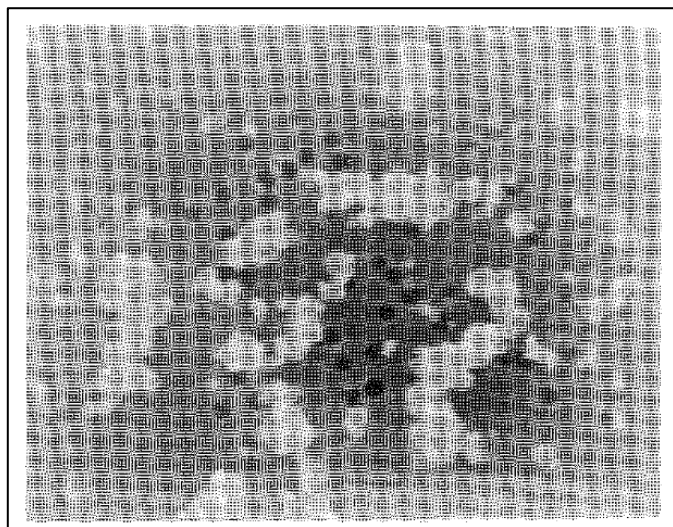


Figure 1. Brockmann and Rader (1990) described this as an "electronmicrograph of cerium oxide particles collected on a nucleopore filter". No scale was indicated in their article.

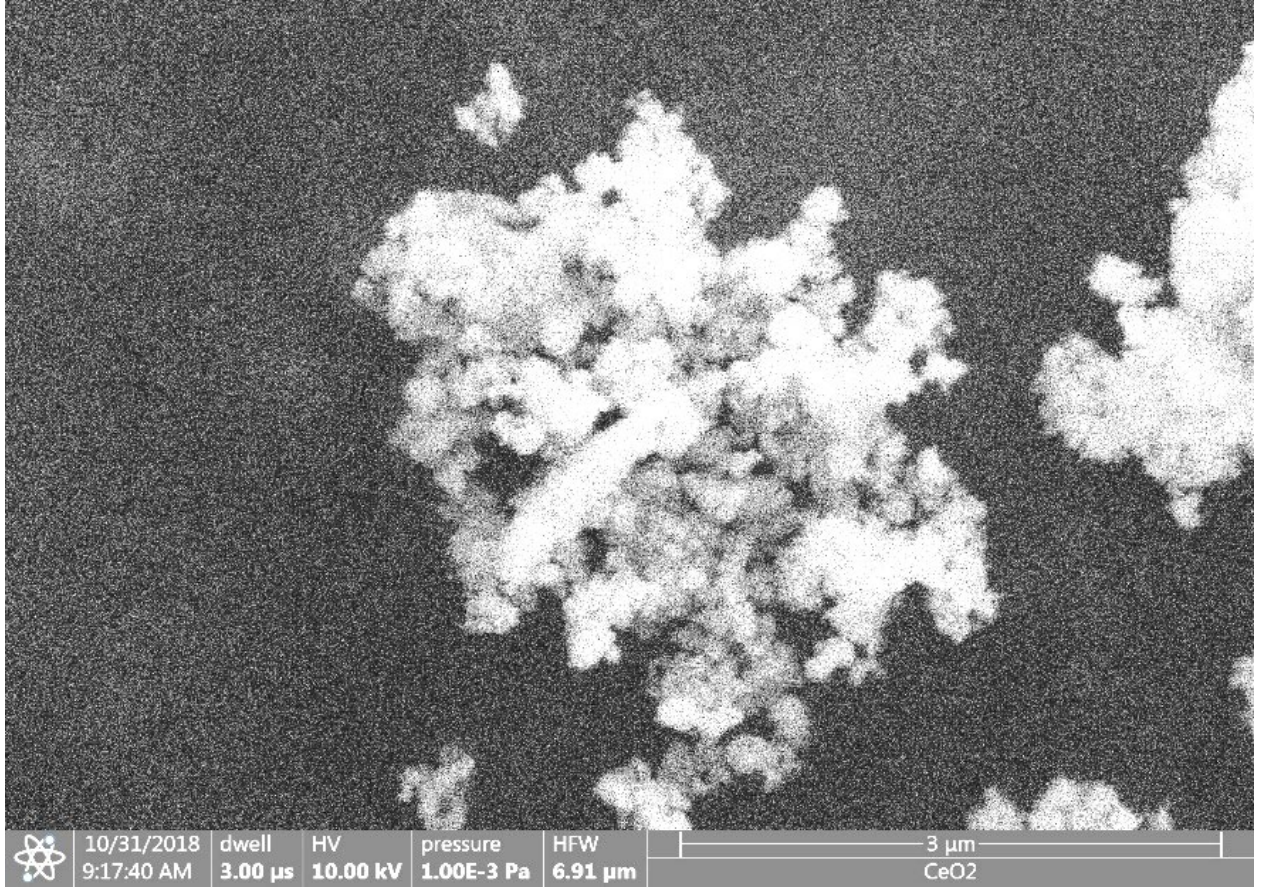


Figure 2. An electron microscope photograph of CeO₂ material in this study. The scale bar corresponds to 3 (three) μm.

While an “ideal” aerosol particle is described as a perfect sphere, a non-spherical particle would be characterized with a dynamic (dimensionless) shape factor (χ) to account for its “non-ideal” shape (Hinds 1999). Aerodynamic diameter is defined as the settling velocity of a spherical particle with unit density, and a non-spherical particle with the same terminal settling velocity (V_{TS}) would be described as:

$$V_{TS} = \frac{\rho_0 d_a^2 g}{18 \mu} = \frac{\rho_P d_P^2 g}{18 \mu \chi_P} = \frac{\rho_B d_B^2 g}{18 \mu \chi_B} \quad (\text{Eq. 1})$$

where,

ρ_0 = unit density of the ideal particle,
 d_a = aerodynamic diameter of the ideal spherical particle,
 g = gravitational acceleration, and
 μ = viscosity of air.

In the Brockmann and Rader work (1990):

ρ_P = physical (maximum) material density of the non-spherical particle (i.e. 7.13 g cm⁻³),
 d_P = equivalent diameter of a sphere with the same volume as the non-spherical particle, and,
 χ_P = dynamic shape factor of the non-spherical particle (cf. Hinds 1999).

In the current approach:

ρ_B = aerated bulk density (i.e. 0.91 g cm⁻¹),

d_B = equivalent volume diameter of a sphere corresponding to the aerated bulk volume, and,

χ_B = dynamic shape factor of the non-ideal (aerated bulk density) particle.

Consider a single hypothetical particle of CeO₂ powder. Its mass could be described by its (ideal) particle properties (subscript P), or by its "bulk" properties (subscript B), where,

$$mass = \frac{\rho_P \pi d_P^3}{6} = \frac{\rho_B \pi d_B^3}{6} \quad (\text{Eq. 2})$$

By algebraic simplification, the shape factor defined by bulk properties (χ_B) in terms of the shape factor (χ_P) (Brockmann and Rader 1990) is:

$$\chi_B = \chi_P \left(\frac{\rho_B}{\rho_P} \right)^{\frac{1}{3}} \quad (\text{Eq. 3})$$

Note there are two definitions for density and shape factor for the exact same particle.

Brockmann and Rader (1990) observed a bimodal aerosol size distribution for CeO₂, with two different shape factors (Table 1). This study conservatively assumes the shape factor (χ =2.66) associated with the smaller size distribution, which is 42% greater than χ =1.87 for the larger aerosol mode.

Table 1. Dynamic shape factor for CeO₂ aerosol particles (Brockmann and Rader 1990).

Aerodynamic equivalent diameter (AED, μm) ranges for the observed bimodal particle size distribution, for a particle density $\rho = 7.13 \text{ g/cc}$.	Shape factor (χ), dimensionless
1 μm to 3 μm	$2.66 \pm 25\%$
3 μm to 10 μm	$1.87 \pm 25\%$

Conclusion

Experimental results that measure $d_a(\mu\text{m})$ (with an Aerodynamic Particle Sizer model APS 3321, TSI Inc, Shoreview MN), the same instrument used by Brockmann and Rader (1990) would yield a value for $d_B(\mu\text{m})$ from a reworking of Equation 1, such that,

$$d_B = d_a \left(\frac{\rho_0}{\rho_B} \chi_B \right)^{1/2} \quad (\text{Eq. 4})$$

For work performed at Los Alamos National Laboratory in the RRFMC (Respirable Release Fraction Measurement Chamber) with an APS 3321, the effective particle diameters of a measured population of aerosol would be computed from the APS 3321 output.

A nominal aerosol with an AED of 10 μm (Table 2) would have an estimated equivalent diameter dependent on the defined shape factor and the density value assigned to the aerosol material, but the estimated mass of a given particle would be identical, regardless of the utilized approach. (Note a slight rounding calculation error is present in Table 2.)

For a given measurement of a particle in an APS 3321 Aerodynamic Particle Sizer, the AED value would also be used to define the appropriate DCF (dose conversion factor), along with the isotopic composition of the particles under consideration.

Table 2. Comparison table for cerium oxide powder (density and shape factor definitions).

	Defined density, g cm⁻³	Nominal d_a, AED (μm)	diameter d_B or d_P (μm)	AED mass (1x10⁻¹² g)	mass (1x10⁻¹² g)	Shape factor
Brockmann and Rader 1990 (d_P)	7.13	10	6.11	523.6	850.7	2.66
Current study (d_B)	0.9114	10	12.13	523.6	851.6	1.34

References

ASTM D7481. 2018. Standard Test Methods for Determining Loose and Tapped Bulk Densities of Powders using a Graduated Cylinder.

Brockmann JE, Rader DJ. APS response to nonspherical particles and experimental determination of dynamic shape factor. *Aerosol Science and Technology*. 1990 Jan 1;13(2):162-72.

Hinds WC. “Aerosol Technology, Properties, Behavior and Measurement of Airborne Particles”, John Wiley and Sons, USA, 2nd ed. 1999

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X: Lucida Calligraphy (capital X)